

On the isotopic shifts in the light two-electron atoms and ions.

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Abstract

The isotopic shifts are determined to high accuracy for a number of light two-electron Li^+ , Be^{2+} , B^{3+} and C^{4+} ions. The field components of these isotopic shifts have been determined with the use of the exact Racah-Rosental-Breit formula.

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The dependence of the total energies of bound states of different isotopes of the same chemical element upon the ‘isotope numbers’ is called the isotopic shift. By the ‘isotope numbers’ we mean the mass of the nucleus and its electric charge density distribution (or proton density distribution). In general, the isotopic shift can be observed in arbitrary, in principle, atomic system which has a central, heavy nucleus with the finite mass, positive electric charge and finite radius. In general, the isotopic shift ΔE of the bound state level with the total energy E has the two following components: the first component which depends upon the mass of the nucleus and the second component which mainly depends upon the electric charge density distribution in the atomic nucleus. In turn, the first component is represented as the sum of the normal and specific components. Each of these two components is proportional to the factor $\frac{m_e}{M}$, where m_e is the mass of the electron, while M is the nuclear mass. For few-electron (N -electron) atoms and ions the exact formula for the isotopic shift ΔE takes the form

$$\Delta E = \Delta E_n + \Delta E_s = \frac{m_e}{M} \left\langle \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m_e} \right\rangle + \frac{m_e}{M} \left\langle \sum_{i(i \neq k)=1}^N \frac{\mathbf{p}_i \cdot \mathbf{p}_k}{2m_e} \right\rangle \quad (1)$$

where the notation $\langle \hat{X} \rangle$ designates the expectation value of the operator \hat{X} . For the two-electron (or helium-like) atoms and ions in atomic units $\hbar = 1, m_e = 1, e = 1$ the last formula is reduced to the form

$$\Delta E = \Delta E_n + \Delta E_s = \frac{1}{M} \langle \mathbf{p}_1^2 \rangle + \frac{1}{2M} \langle \mathbf{p}_1 \cdot \mathbf{p}_2 \rangle \quad (2)$$

As follows from this formula the expression for the normal and specific components of the isotopic shift are

$$\Delta E_n = \frac{1}{M} \langle \mathbf{p}_1^2 \rangle \quad \text{and} \quad \Delta E_s = \frac{1}{2M} \langle \mathbf{p}_1 \cdot \mathbf{p}_2 \rangle \quad , \quad (3)$$

respectively. As follows from Eq.(3) to determine the normal and specific components of the isotopic shift in two-electron atom/ion one needs to obtain the expectation values of the \mathbf{p}_1^2 and $\mathbf{p}_1 \cdot \mathbf{p}_2$ operators. Everywhere in this study we assume that the wave functions of the two-electron atom/ion are properly symmetrized upon spin-spatial permutations of the two electrons and, therefore, the corresponding single-electron expectation values are always equal to each other, e.g., $\langle \mathbf{p}_1^2 \rangle = \langle \mathbf{p}_2^2 \rangle$.

In actual two-electron atomic systems, i.e. in the systems with the finite nuclear mass M , one can use the condition which follows from the conservation of the total momentum

$\mathbf{P}_N = \mathbf{p}_1 + \mathbf{p}_2$, where \mathbf{P}_N is the momentum of the nucleus, while \mathbf{p}_1 and \mathbf{p}_2 are the electron momenta. From here one finds:

$$\frac{1}{2}\langle \mathbf{P}_N^2 \rangle = \langle \mathbf{p}_1^2 \rangle + \langle \mathbf{p}_1 \cdot \mathbf{p}_2 \rangle \quad (4)$$

and, therefore, from Eqs.(2) and (4) we have

$$\Delta E = \frac{1}{2M} \langle \mathbf{P}_N^2 \rangle \quad (5)$$

i.e. the mass dependent component of the isotopic shift is the expectation value of the kinetic energy of the atomic nucleus with the large (but finite!) mass. In many books and textbooks the formula, Eq.(5), is considered as the original (or fundamental) expression, while Eq.(1) is derived from this formula.

As mentioned above the field component of the isotopic shift explicitly depends upon the nuclear size (radius) R and proton distribution density in the nucleus. It is clear that this component also depends upon the mass of atomic nucleus M , since the nuclear matter is a saturated matter (in contrast with the Coulomb matter). Therefore, the nuclear radius R is uniformly related to the number of nucleons A in the nucleus: $R = r_0 \cdot A^{\frac{1}{3}}$, where the ‘constant’ radius $r_0 \approx 1.17 - 1.25 \cdot 10^{-13} \text{ cm} = 1.17 - 1.25 \text{ fm}$ (fermi), where $1 \text{ fm} = 1 \cdot 10^{-13} \text{ cm}$. Briefly, this means that the field component of the total isotopic shift is also a function of the nuclear mass M , since $A \approx \frac{M}{m_p}$, where m_p is the proton mass. The more accurate formula for the nuclear mass as the function of $A, Z(= N_p)$, where Z is the electric charge of the nucleus = number of protons N_p and N_n (number of neutrons) is given by the Weizäcker formula. This formula is discussed in the Appendix.

Let us present here the well known formula obtained by Racah, Rosental and Breit for the field shift (see, e.g., [1] and references therein)

$$E_M^{fs} = \frac{4\pi a_0^2}{Q} \cdot \frac{b+1}{[\Gamma(2b+1)]^2} \cdot B(b) \cdot \left(\frac{2QR}{a_0}\right)^{2b} \cdot \frac{\delta R}{R} \cdot \langle \delta(\mathbf{r}_{eN}) \rangle \quad (6)$$

where Q is the nuclear charge, R is the nuclear radius and $b = \sqrt{1 - \alpha^2 Q^2}$, where $\alpha = \frac{e^2}{\hbar c} \approx \frac{1}{137}$ is the dimensionless constant which is the small parameter in QED. In Eq.(3) the notation $\Gamma(x)$ stands for the Euler’s gamma-function, while the factor $B(b)$ is directly related to the proton density distribution in the atomic nucleus. By assuming the uniform distribution of the proton density over the volume of the nucleus one finds the following expression for the factor $B(b)$

$$B(b) = \frac{3}{(2b+1)(2b+3)} \quad (7)$$

For light nuclei with $Q \leq 6$ we have $b \approx 1$ and $B \approx \frac{1}{5}$. The formula, Eq.(6), was used in many theoretical papers for numerical evaluations of the field component of the isotopic shift, or field shift for short. In some works, however, this formula was written with a number of ‘obvious simplifications’. Many of such ‘simplifications’ are based on the fact that for light nuclei the numerical value of the factor b is close to unity. Furthermore, in some papers the factor b was mistakenly called and considered as the Lorentz factor, while the actual Lorentz factor γ is its inverse value $\gamma = \frac{1}{b} = \frac{1}{\sqrt{1-\alpha^2 Q^2}}$. Such a factor γ always exceeds unity.

In this study we evaluate the isotopic shift for a number of the ground $1^1S(L=0)$ -states in the light two-electron ions by using the exact (not approximate!) formula, Eq.(6). Such evaluations allow one to evaluate the numerical errors which arise from the use of approximate expressions. Our main interest in this study is related with the field component of the isotopic shift. As follows from Eq.(6) to evaluate the field component of the field shift one needs to determine to very high accuracy the expectation value of the electron-nuclear delta-function (or the $\langle \delta(\mathbf{r}_{eN}) \rangle$ value). In this study for each light element/atom all isotopic shifts are determined in respect to the model (or idealized) isotope which has the infinitely heavy nucleus with zero spatial radius (zero charged radius). In this case the ratio $\frac{\delta R}{R}$ in Eq.(6) equals unity, and this equation can be re-written to the form (in atomic units)

$$E_M^{fs} = 4^{b+1} \pi Q^{2b-1} \cdot \alpha^{4b} \cdot \frac{3(b+1)}{[\Gamma(2b+1)]^2 (2b+1)(2b+3)} \cdot \left(\frac{R}{r_e}\right)^{2b} \cdot \langle \delta(\mathbf{r}_{eN}) \rangle \quad (8)$$

where $r_e = \alpha^2 a_0 \approx 2.817940 \text{ fm}$ ($1 \text{ fm} = 10^{-13} \text{ cm}$) is the classical radius of the electron. For light atomic nuclei the dimensionless factor $\frac{R}{r_e}$ in the last formula is close to unity. Also, in our calculations we have used the following numerical values for the physical constants: $\alpha = 7.297352569 \cdot 10^{-3}$ and $a_0 = 5.291772109 \cdot 10^{-9} \text{ cm}$. The formula, Eq.(8), has been used in all calculations performed for this study. As follows from Eq.(8) to determine the field component of the isotopic shift one needs to know the expectation value of the electron-nuclear delta-function $\delta(\mathbf{r}_{eN})$ and numerical value of the nuclear radius R . The expectation value of $\delta(\mathbf{r}_{eN})$ can be found from the results of highly accurate atomic computations, while the nuclear radius must be taken from nuclear experiments (see, e.g., [6]).

In this study we consider a few light two-electron (or He-like) ions: Li^+ , Be^{2+} , B^{3+} and C^{4+} . The total energies and some other properties (or expectation values) of the corresponding model ions (with the infinite nuclear mass and zero spatial radii) can be found in Tables I - IV. The convergence of the results upon the total number of basis function N

used in calculations is also shown in Tables I - IV. For these Tables we have computed the expectation values of the following operators: $\delta(\mathbf{r}_{eN})$, ν_{eN} , \mathbf{p}_1^2 , $\mathbf{p}_1 \cdot \mathbf{p}_2$ and \mathbf{p}_N^2 . The notation ν_{eN} designates the electron-nuclear cusp value which is defined by the following equation

$$\nu_{eN} = \frac{\langle \delta(\mathbf{r}_{eN}) \frac{\partial}{\partial r_{eN}} \rangle}{\langle \delta(\mathbf{r}_{eN}) \rangle} \quad (9)$$

Formally, it is an averaged velocity of the electron at the nucleus. In the general case, this expectation value gives the relative velocity of the two particles (i and j) at the (ij) -collision point. For pure Coulomb systems, e.g., for the atom with the nuclear charge Q , such a velocity is known from the corresponding classical problem. In particular, for the atom with the nuclear charge Q , the electron-nuclear cusp ν_{eN} must be equal (in atomic units)

$$\nu_{eN} = -Qe^2 \frac{m_e M_N}{m_e + M_N} = -Q \quad (10)$$

since $M_N = \infty$.

The coincidence of the computed ν_{eN} value with the nuclear charge Q (or $-Q$) indicates the quality of the variational (atomic) wave functions around the nucleus and overall accuracy of the computed expectation value of the electron-nuclear delta-function. In all calculations performed for this study we have used our exponential variational expansion in relative coordinates described in detail in our earlier papers, see, e.g., [2], [3]. Here we do not want to repeat these descriptions of our variational expansion. Note also that in our calculations we have determined many dozens of different expectation values, including singular expectation values. However, in Tables I - IV only a few expectation values are presented. All these values are needed for numerical evaluation of the isotopic shifts.

Table V contains the numerical values of the field components of isotopic shifts (in *a.u.*) determined with the use of the formula Eq.(8). In this Table we also present the numerical values of the following factors from that formula: R (the actual nuclear radius), b , $X = 4^{b+1} \pi Q^{2b-1} \cdot \alpha^{4b} \cdot \frac{3(b+1)}{[\Gamma(2b+1)]^2 (2b+1)(2b+3)}$ and $Y = \left(\frac{R}{r_e}\right)^{2b}$. The expectation values of the electron-nuclear delta-functions were taken from Tables I - IV. To evaluate the Euler's gamma-function $\Gamma(x)$ we have used the approximate 7-term formula derived by Lanczos [7]. The overall accuracy of this formula is $\approx 1 \cdot 10^{-10} - 2 \cdot 10^{-10}$.

Appendix I.

The formula which provides the uniform relation between the nuclear mass M and total number of nucleons A , nuclear charge Z (= number of protons N_p) and number of neutrons

N_n in the nucleus was derived in 1937 by Bethe, Weizäcker and others. Now, this formula is known as the Weizäcker formula [8], or Bethe-Weizäcker formula. This five-term formula for the nuclear binding energy E_b was produced 75 years ago and since then its general structure has never been changed. First, note that the mass formula for an arbitrary nucleus is written in the form

$$M = m_p \left[Z + N \left(\frac{m_n}{m_p} \right) - \frac{E_b}{m_p c^2} \right] \quad (11)$$

where M is the nuclear mass of the nucleus with A nucleons, Z protons and N neutrons ($A = Z + N$). Also in this formula E_b is the binding energy of the nucleus, c is the speed of light in vacuum, while m_p and m_n are the masses of the proton and neutron, respectively. The factors $m_p c^2 = 938.272910 \text{ MeV}$ and $m_n c^2 = 939.565378 \text{ MeV}$. The advantage of the formula, Eq.(11), is obvious, since it contains only dimensionless ratios and two integer numbers (Z and N). For instance, if we chose in Eq.(11) $m_p = 1836.152701 m_e$, then M will be given in m_e (or in atomic units if $m_e = 1$). This is very convenient for highly accurate computations of different few-electron ions.

The parameter E_b in Eq.(11) is called the binding energy of the nucleus. The explicit expression for the nuclear binding energy E_b is written as the following sum (the Weizäcker formula):

$$E_b = a_V A - a_S A^{\frac{2}{3}} - a_C \frac{Z^2}{A^{\frac{1}{3}}} - a_A \frac{(N - Z)^2}{A} + \delta(A, Z) \quad (12)$$

where the five terms in the right-hand side of this equation are called the volume term, surface term, Coulomb term, asymmetry term and pairing term, respectively. The pairing term $\delta(A, Z)$ equals zero, if A is odd. If A is even and both Z and N are even, then $\delta(A, Z) = \frac{a_p}{\sqrt{A}}$. The Weizäcker formula is relatively accurate for regular nuclei (i.e. for nuclei which are not far from the stability region). In reality, such an accuracy directly depends upon the numerical values of parameters a_V, a_S, a_C, a_A and a_p in Eq.(12). In our calculations we have used the following values of these parameters: $a_V = 15.8 \text{ MeV}$, $a_S = 18.3 \text{ MeV}$, $a_C = 0.714 \text{ MeV}$, $a_A = 23.2 \text{ MeV}$ and $a_p = 12.0 \text{ MeV}$. The Weizäcker formula with these coefficients is sufficiently accurate for all light nuclei which are located in the stability region.

Appendix II.

In general, the bound state in any few-electron atom arises in the result of proper balance between kinetic energy T_e of atomic electrons, electron-nuclear (Coulomb) attraction U_{en} and

electron-electron (Coulomb) repulsion U_{ee} . The total energy E of this bound state is written as the following sum:

$$E = T_e + U_{ne} + U_{ee} = \frac{1}{2}(U_{ne} + U_{ee}) \quad (13)$$

where in the right-hand side we have used the virial theorem for the Coulomb potential (see, e.g., [9]) $T_e = -\frac{1}{2}(U_{ne} + U_{ee})$. To solve the problem we need the explicit expression for the correlation energy U_{ee} in terms of the electron-nuclear attraction energy U_{ne} . Such an analytical relation can be found in a few restricted cases, e.g., in the Thomas-Fermi method one finds: $U_{ee} = -\frac{1}{7}U_{ne}$ and $E = \frac{3}{7}U_{ne}$. For highly accurate method the situation is significantly more complicated, but qualitatively the actual relations between T_e , U_{ne} and U_{ee} are similar to the relations obeyed in the Thomas-Fermi model.

First, note that the Schrödinger equation for an arbitrary non-relativistic N -electron atom/ion takes the form

$$\left[\frac{\hbar^2}{2m_e} \sum_{i=1}^N \mathbf{p}_i^2 - Qe^2 \sum_{i=1}^N \frac{1}{r_i} + e^2 \sum_{i>j=1}^N \frac{1}{r_{ij}} \right] \Psi = E\Psi \quad (14)$$

where Q is the electric charge of the nucleus and the mass of the central nucleus is assumed to be finite. Here we shall not assume that $N = Q$. In Eq.(14) the terms in the first sum ($\sim \mathbf{p}_i^2$) represent the kinetic energies of electrons, while other terms correspond to the electron-nuclear Coulomb attraction and/or electron-electron Coulomb repulsion. From this equation one finds the following relation for the expectation values (in atomic units):

$$\left[\frac{N}{2} \langle \mathbf{p}_e^2 \rangle - QN \langle \frac{1}{r_{en}} \rangle + \frac{N(N-1)}{2} \langle \frac{1}{r_{ee}} \rangle \right] = E \quad (15)$$

where the subscript e means the electron, while the subscript n stands for the nucleus.

Let us assume that we know the highly accurate solution of the Schrödinger equation, i.e. the wave function Ψ in Eq.(14) is known. In this case the following condition must be obeyed for these three expectation values:

$$\langle \mathbf{p}_e^2 \rangle = Q \langle \frac{1}{r_{en}} \rangle - \frac{(N-1)}{2} \langle \frac{1}{r_{ee}} \rangle \quad (16)$$

which is known as the virial theorem (see, e.g., [9]). Now, after a few steps of simple transformations one finds the following formula for the total energy E (in atomic units)

$$\begin{aligned} E &= -\frac{1}{2}N \cdot Q \cdot \langle \frac{1}{r_{en}} \rangle + \frac{1}{4}N(N-1) \cdot \langle \frac{1}{r_{ee}} \rangle \\ &= -\frac{1}{2}N \cdot Q \cdot f_1(N, Q) + \frac{1}{4}N(N-1) \cdot f_2(N, Q) \end{aligned} \quad (17)$$

where $f_1(N, Q)$ and $f_2(N, Q)$ are the functions of the number of electrons N and electric charge of the nucleus Q . For neutral atoms we have $Q = N$, while for positively charged ions $Q > N$. For instance for the two-electron C^{4+} ion (i.e. for $N = 2$ and $Q = 6$) we found that $\langle \frac{1}{r_{en}} \rangle \approx 5.687615325399107305988929 \text{ a.u.}$ and $\langle \frac{1}{r_{ee}} \rangle \approx 3.438890700992227050791016158 \text{ a.u.}$ (results from calculations with 3700 basis functions). By using these expectation values one finds the total energy E from Table IV. In the general case, $\langle \frac{1}{r_{ee}} \rangle = \lambda(N, Q) \langle \frac{1}{r_{en}} \rangle$, where the parameter $\lambda < 1$. The factor $\lambda(N, Q)$ can be approximated to very high accuracy with the use of highly accurate results obtained for different N and Q .

The formula, Eq.(17), is also applied in the case of $N = 1$ (hydrogen-like atoms and ions). In this case the electron-electron repulsion is not defined, but it is multiplied by a factor which equals zero. As follows from Eq.(17), if we can determine the two unknown functions $f_1(N, Q)$ and $f_2(N, Q)$ in Eq.(17), then we can predict the total energy of an arbitrary N -electron atom/ion to very high accuracy. It can be done, e.g., by using the results of highly accurate computations of different few-electron atoms and ions (with different Q and N). If we know the results of highly accurate computations for a large number of light atoms/ions, then we can reconstruct the two functions $f_1(N, Q)$ and $f_2(N, Q)$ in Eq.(17) to very high accuracy. This procedure works well for mixtures of light elements at different temperatures and allows one to predict the properties of high-temperature plasmas which consists of such elements.

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TABLE I: The total energies E and expectation values of the electron-nuclear delta-function δ_{eN} , electron-nuclear cusp ν_{eN} and some other operators for the two-electron lithium ion Li^+ (in atomic units). K is the total number of basis functions used.

K	$E(\text{Li}^+)$					$\langle\delta_{eN}\rangle$			ν_{eN}				
3500	-7.279913	412669	305964	91708		6.8520	094343	431	-3.0000	00000	158		
3700	-7.279913	412669	305964	91743		6.8520	094343	456	-3.0000	00000	125		
3840	-7.279913	412669	305964	91766		6.8520	094343	460	-2.9999	99999	918		
4000	-7.279913	412669	305964	91785		6.8520	094343	462	-2.9999	99999	901		
K	$\frac{1}{2}\langle\mathbf{p}_1^2\rangle$					$\langle\mathbf{p}_1\cdot\mathbf{p}_2\rangle$			$\frac{1}{2}\langle\mathbf{p}_N^2\rangle$				
3500	3.63995	670633	465298	240		0.288975	786393	989535	661	7.56888	919906	329532	141
3700	3.63995	670633	465298	241		0.288975	786393	989535	661	7.56888	919906	329532	143
3840	3.63995	670633	465298	241		0.288975	786393	989535	662	7.56888	919906	329532	144
4000	3.63995	670633	465298	242		0.288975	786393	989535	662	7.56888	919906	329532	145

TABLE II: The total energies E and expectation values of the electron-nuclear delta-function δ_{eN} , electron-nuclear cusp ν_{eN} and some other operators for the two-electron berillium ion Be^{2+} (in atomic units). K is the total number of basis functions used.

K	$E(\text{Be}^{2+})$					$\langle\delta_{eN}\rangle$				ν_{eN}			
3500	-13.65556	623842	358670	20757		17.1981	72544	645		-3.9999	99999	962	
3700	-13.65556	623842	358670	20767		17.1981	72544	640		-3.9999	99999	921	
3840	-13.65556	623842	358670	20772		17.1981	72544	638		-4.0000	00000	125	
4000	-13.65556	623842	358670	20777		17.1981	72544	635		-4.0000	00000	148	
K	$\frac{1}{2}\langle\mathbf{p}_1^2\rangle$					$\langle\mathbf{p}_1\cdot\mathbf{p}_2\rangle$				$\frac{1}{2}\langle\mathbf{p}_N^2\rangle$			
3500	6.82778	311921	179335	084		0.420520	303439	441862	011	14.07608	654186	302856	368
3700	6.82778	311921	179335	086		0.420520	303439	441862	010	14.07608	654186	302856	369
3840	6.82778	311921	179335	089		0.420520	303439	441862	009	14.07608	654186	302856	370
4000	6.82778	311921	179335	091		0.420520	303439	441862	009	14.07608	654186	302856	371

TABLE III: The total energies E and expectation values of the electron-nuclear delta-function δ_{eN} , electron-nuclear cusp ν_{eN} and some other operators for the two-electron boron ion B^{3+} (in atomic units). K is the total number of basis functions used.

K	$E(B^{3+})$					$\langle \delta_{eN} \rangle$				ν_{eN}			
3500	-22.03097	1580242	781541	65339		34.758	743660	955		-5.0000	0000	319	
3700	-22.03097	1580242	781541	65376		34.758	743660	965		-5.0000	0000	235	
3840	-22.03097	1580242	781541	65394		34.758	743660	947		-5.0000	0000	107	
4000	-22.03097	1580242	781541	65418		34.758	743660	935		-5.0000	0000	119	
K	$\frac{1}{2}\langle \mathbf{p}_1^2 \rangle$					$\langle \mathbf{p}_1 \cdot \mathbf{p}_2 \rangle$				$\frac{1}{2}\langle \mathbf{p}_N^2 \rangle$			
3500	11.01548	579012	139077	100		0.552752	631642	101467	789	22.58372	421188	488300	979
3700	11.01548	579012	139077	089		0.552752	631642	101467	734	22.58372	421188	488300	952
3840	11.01548	579012	139077	086		0.552752	631642	101467	715	22.58372	421188	488300	942
4000	11.01548	579012	139077	083		0.552752	631642	101467	701	22.58372	421188	488300	938

TABLE IV: The total energies E and expectation values of the electron-nuclear delta-function δ_{eN} , electron-nuclear cusp ν_{eN} and some other operators for the two-electron carbon ion C^{4+} (in atomic units). K is the total number of basis functions used.

K	$E(\text{C}^{4+})$					$\langle\delta_{eN}\rangle$			ν_{eN}		
3500	-32.40624	660189	853031	05527		61.443	578056	445	-5.9999	99998	765
3700	-32.40624	660189	853031	05535		61.443	578056	514	-5.9999	99999	871
3840	-32.40624	660189	853031	05539		61.443	578056	537	-6.0000	00000	048
4000	-32.40624	660189	853031	05542		61.443	578056	543	-6.0000	00000	037

K	$\frac{1}{2}\langle\mathbf{p}_1^2\rangle$					$\langle\mathbf{p}_1\cdot\mathbf{p}_2\rangle$				$\frac{1}{2}\langle\mathbf{p}_N^2\rangle$			
3500	16.20312	330094	926515	523		0.685334	822135	598924	527	33.09158	142403	412923	500
3700	16.20312	330094	926515	524		0.685334	822135	598924	535	33.09158	142403	412923	502
3840	16.20312	330094	926515	525		0.685334	822135	598924	536	33.09158	142403	412923	502
4000	16.20312	330094	926515	525		0.685334	822135	598924	537	33.09158	142403	412923	503

TABLE V: The nuclear radius R (fm), parameter b , factors X and Y (see the main text) and field components of the total isotopic shift ΔE^{fs} (all values are in atomic units) for each isotope.

isotope	Q	R	b	X	Y	ΔE^{fs}
${}^6\text{Li}$	3	2.5385	0.99976034018621	$4.297056149289 \cdot 10^{-8}$	0.81154478	$2.389469390 \cdot 10^{-7}$
${}^7\text{Li}$	3	2.4312	0.99976034018621	$4.297056149289 \cdot 10^{-8}$	0.74440369	$2.191782729 \cdot 10^{-7}$
${}^9\text{Be}$	4	2.5180	0.99957389838248	$5.749782211793 \cdot 10^{-8}$	0.79852685	$7.896292299 \cdot 10^{-7}$
${}^{10}\text{B}$	5	2.4278	0.99933413638122	$7.219245621776 \cdot 10^{-8}$	0.74241787	$1.862963331 \cdot 10^{-6}$
${}^{11}\text{B}$	5	2.4059	0.99933413638122	$7.219245621776 \cdot 10^{-8}$	0.72909310	$1.829527229 \cdot 10^{-6}$
${}^{12}\text{C}$	6	2.4073	0.99904101579314	$8.7092766851788 \cdot 10^{-8}$	0.76867983	$4.113429628 \cdot 10^{-6}$
${}^{13}\text{C}$	6	2.4614	0.99904101579314	$8.7092766851788 \cdot 10^{-8}$	0.76315629	$4.083871553 \cdot 10^{-6}$
${}^{14}\text{C}$	6	2.5037	0.99904101579314	$8.7092766851788 \cdot 10^{-8}$	0.78958608	$4.225305034 \cdot 10^{-6}$